

QUDA ON GPUS

March 2016
Brookhaven National Laboratory

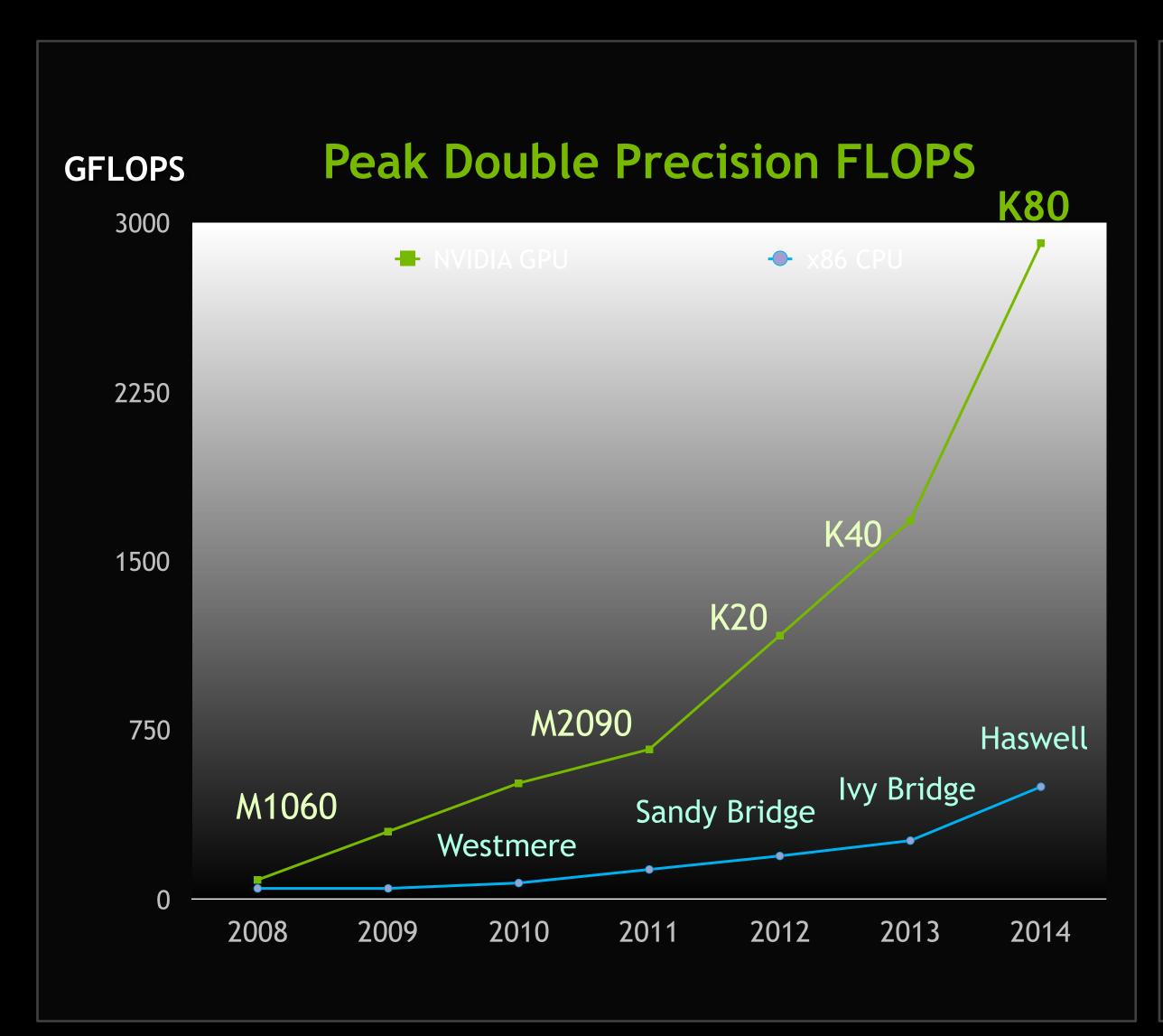
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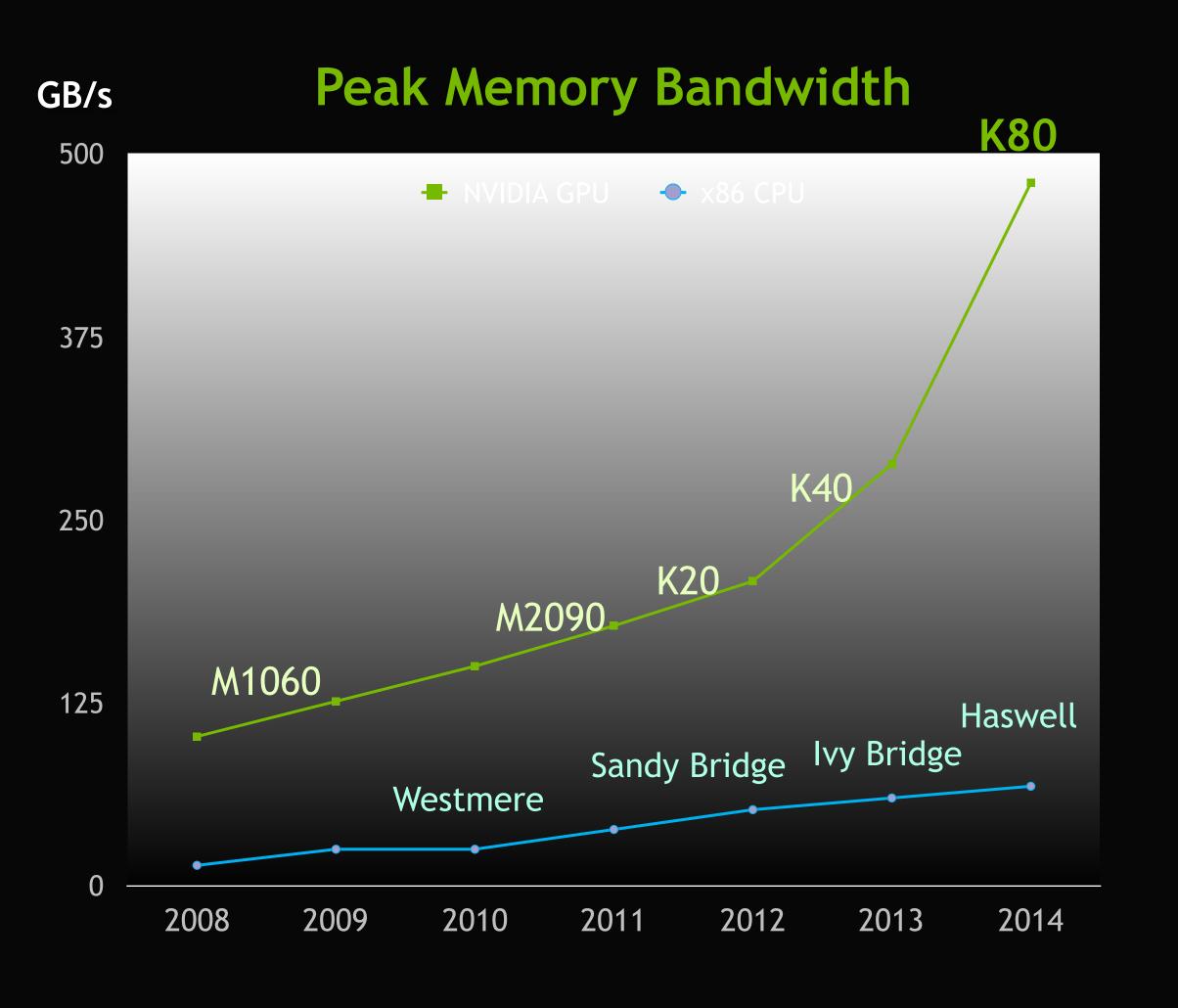
GPUs

QUDA

Multigrid and Hierarchical Algorithms

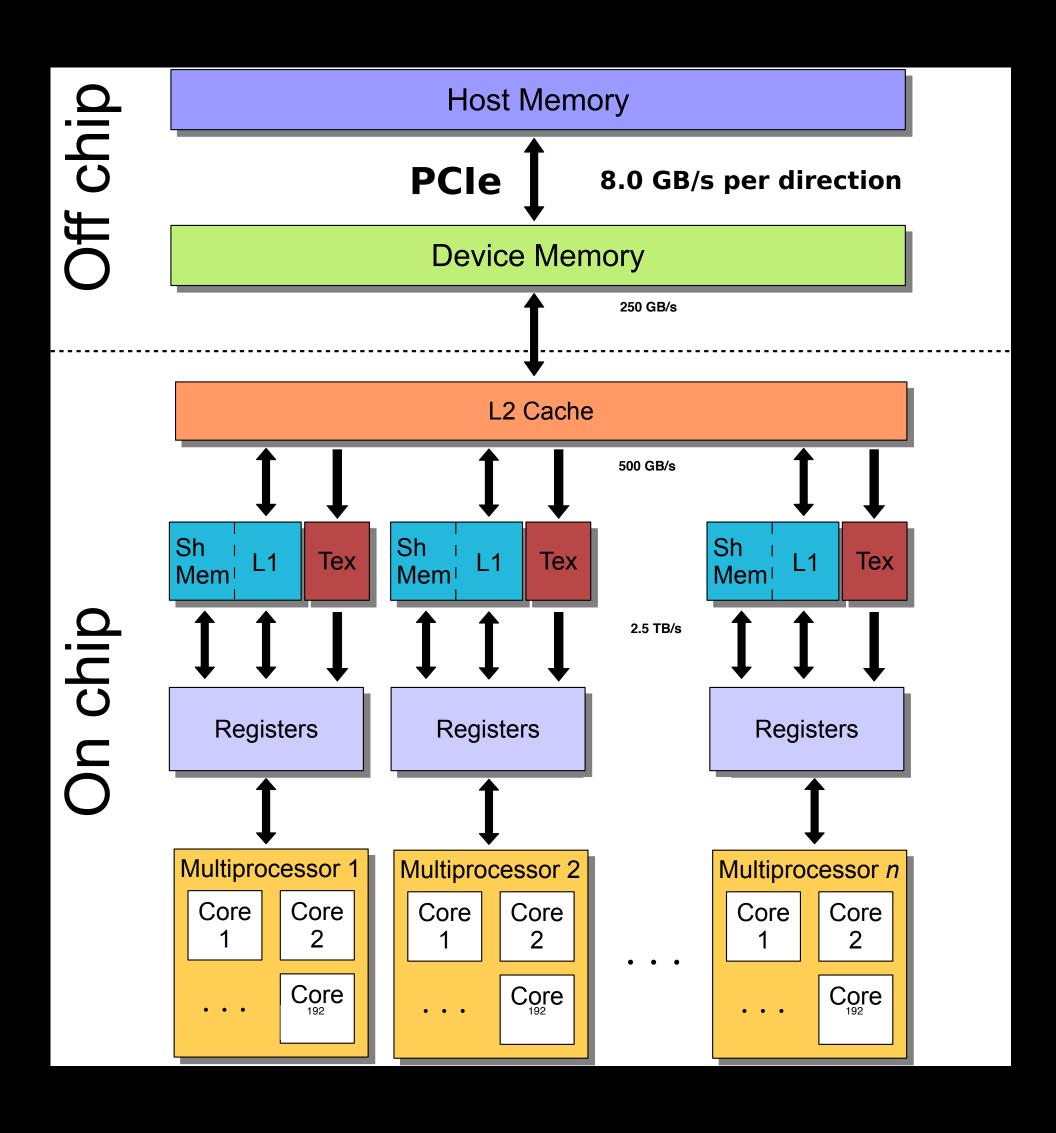
Exascale

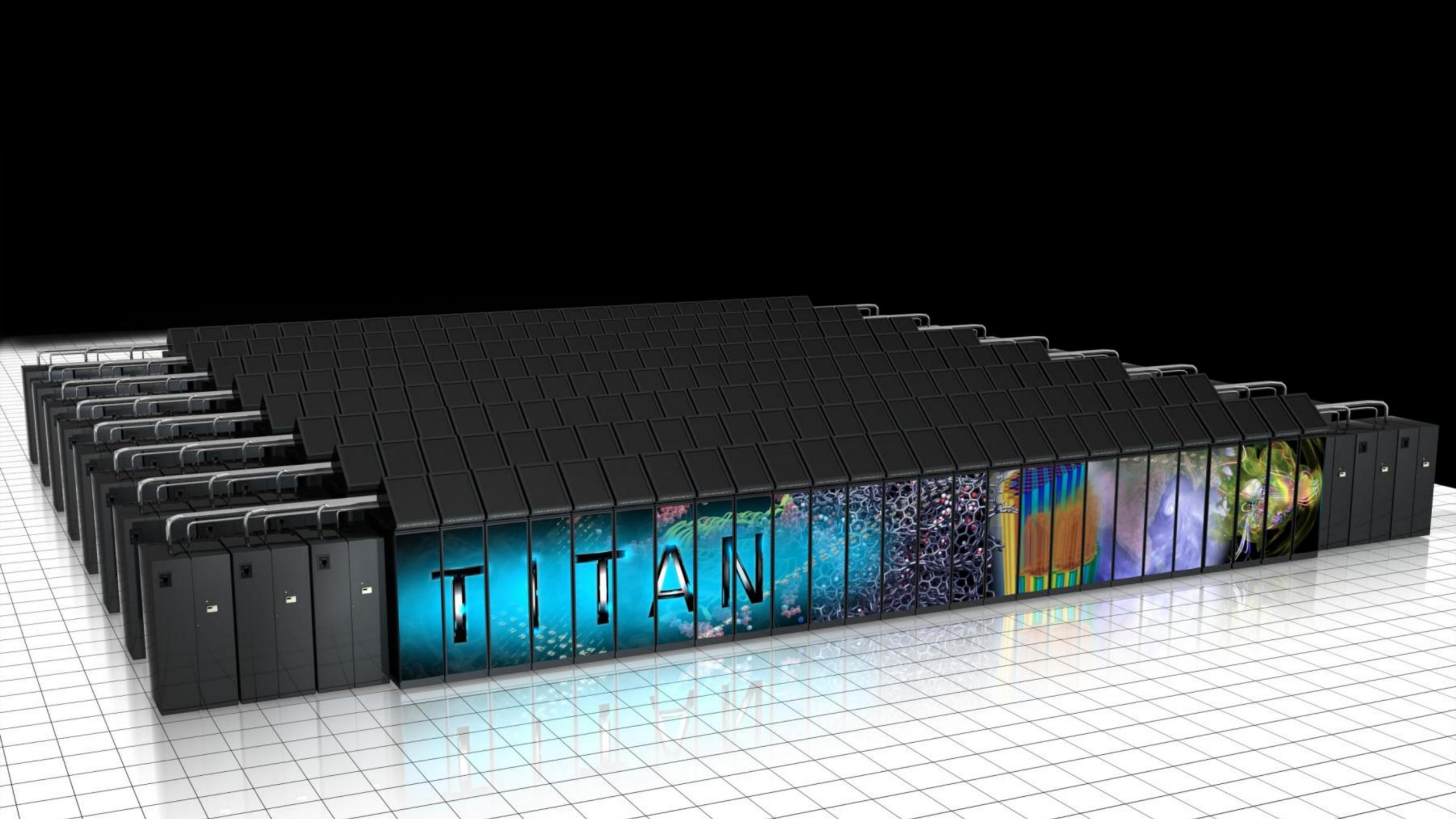




What is a GPU?

- Kepler K20X (2012)
 - 2688 processing cores
 - 3995 SP Gflops peak
- Effective SIMD width of 32 threads (warp)
- Deep memory hierarchy
- As we move away from registers
 - Bandwidth decreases
 - Latency increases
- Programmed using a thread model
 - Architecture abstraction is known as CUDA
 - Fine-grained parallelism required
- Diversity of programming languages
 - CUDA C/C++/Fortran
 - OpenACC, OpenMP 4.0
 - Python, etc.



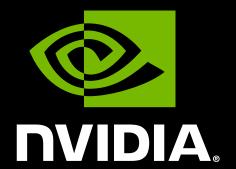


QUDA









- "QCD on CUDA" http://lattice.github.com/quda (open source)
- Effort started at Boston University in 2008, now in wide use as the GPU backend for BQCD, Chroma, CPS, MILC, TIFR, tmQCD, etc.
 - Latest release 0.8.0 (8th February 2016)
- Provides:
 - Various solvers for all major fermionic discretizations, with multi-GPU support
 - Additional performance-critical routines needed for gauge-field generation
 - Gauge fixing, pure gauge evolution, link smearing, etc.
- Maximize performance
 - Exploit physical symmetries to minimize memory traffic
 - Mixed-precision methods
 - Autotuning for high performance on all CUDA-capable architectures
 - Domain-decomposed (Schwarz) preconditioners for strong scaling
 - Eigenvector and deflated solvers (Lanczos, EigCG, GMRES-DR)
 - Multigrid solvers for optimal convergence
- A research tool for how to reach the exascale

In the QUDA Pipeline

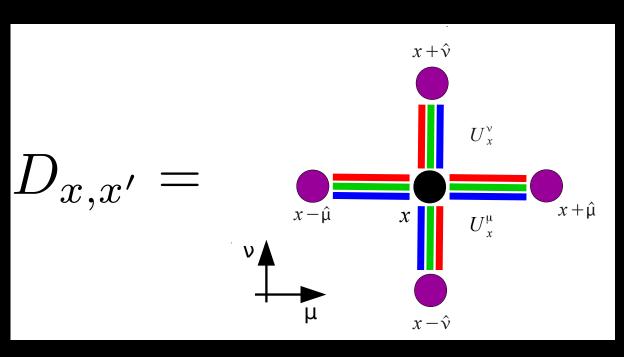
- Dramatically improved 4-d domain-wall performance
- Drastically improved strong scaling
 - Intra node direct communication between GPUs (no MPI)
 - GPU Direct Async NIC and GPU can synchronize with no CPU
- Improved deflation algorithms
- Stout smearing
- Multi-right-hand-side solvers
- Communication avoiding solvers (s-step)
- Improved reduction support (including quad-precision)

QUDA collaborators

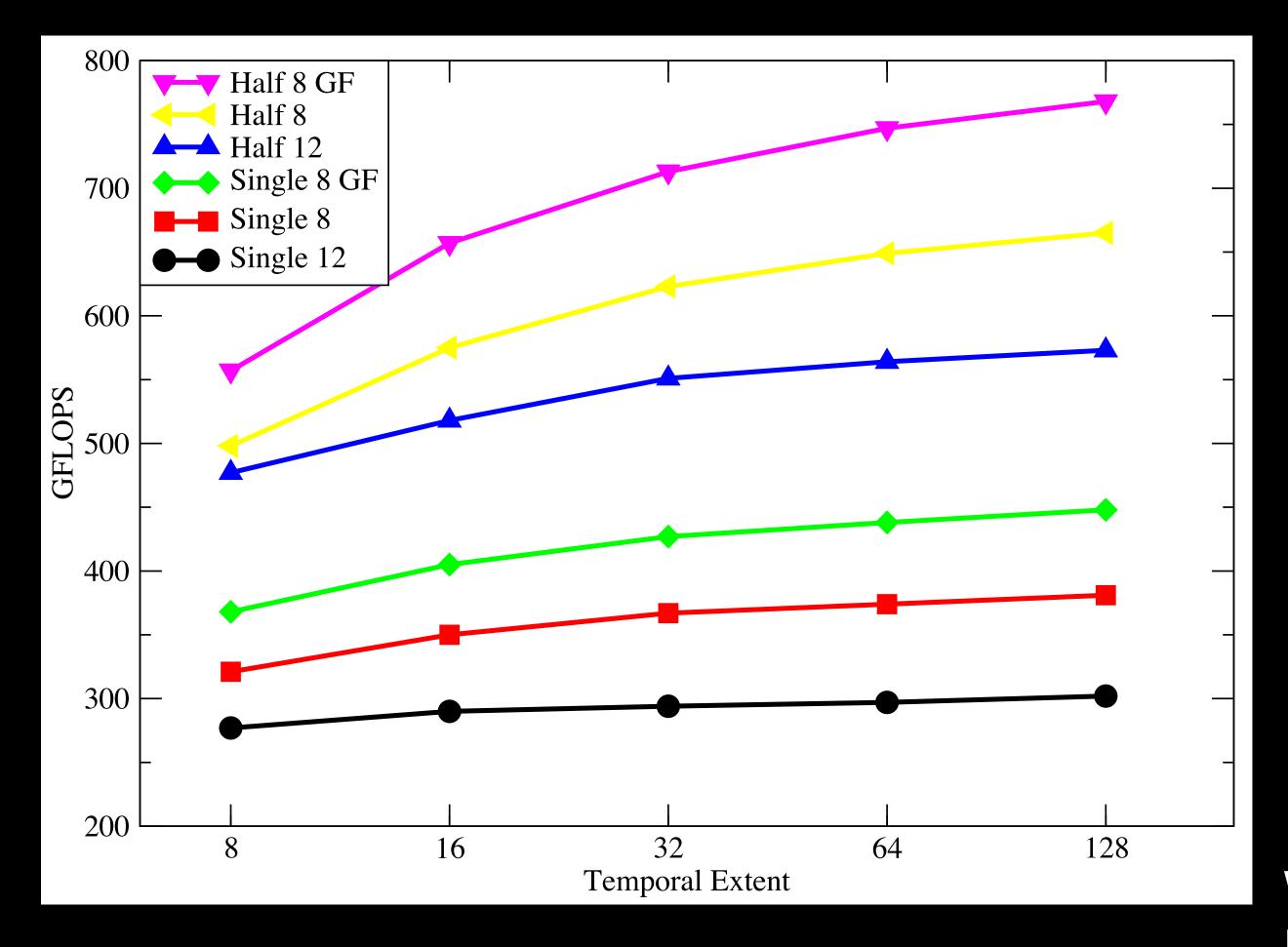
- Ron Babich (NVIDIA)
- Michael Baldhauf (Regensburg)
- Kip Barros (LANL)
- Rich Brower (Boston University)
- Nuno Cardoso (NCSA)
- Michael Cheng (Boston University)
- Carleton DeTar (Utah University)
- Justin Foley (Utah -> NIH)
- Joel Giedt (Rensselaer Polytechnic Institute)
- Steve Gottlieb (Indiana University)
- Bálint Joó (Jlab)
- Hyung-Jin Kim (BNL -> Samsung)
- Claudio Rebbi (Boston University)
- Guochun Shi (NCSA -> Google)
- Mario Schröck (INFN)
- Alexei Strelchenko (FNAL)
- Alejandro Vaquero (INFN)
- Mathias Wagner (NVIDIA)
- Frank Winter (Jlab)

Mapping the Dirac operator to CUDA

- Finite difference operator in LQCD is known as Dslash
- Assign a single space-time point to each thread
 - V = XYZT threads, e.g., $V = 24^4 => 3.3 \times 10^6$ threads
- Looping over direction each thread must
 - Load the neighboring spinor (24 numbers x8)
 - Load the color matrix connecting the sites (18 numbers x8)
 - Do the computation
 - Save the result (24 numbers)
- Each thread has (Wilson Dslash) 0.92 naive arithmetic intensity
- QUDA reduces memory traffic
 - Exact SU(3) matrix compression (18 => 12 or 8 real numbers)
 - Similarity transforms to increase operator sparsity
 - Use 16-bit fixed-point representation
 - No loss in precision with mixed-precision solver
 - Almost a free lunch (small increase in iteration count)



Kepler Wilson-Dslash Performance



Wilson Dslash K20X performance $V = 24^3xT$

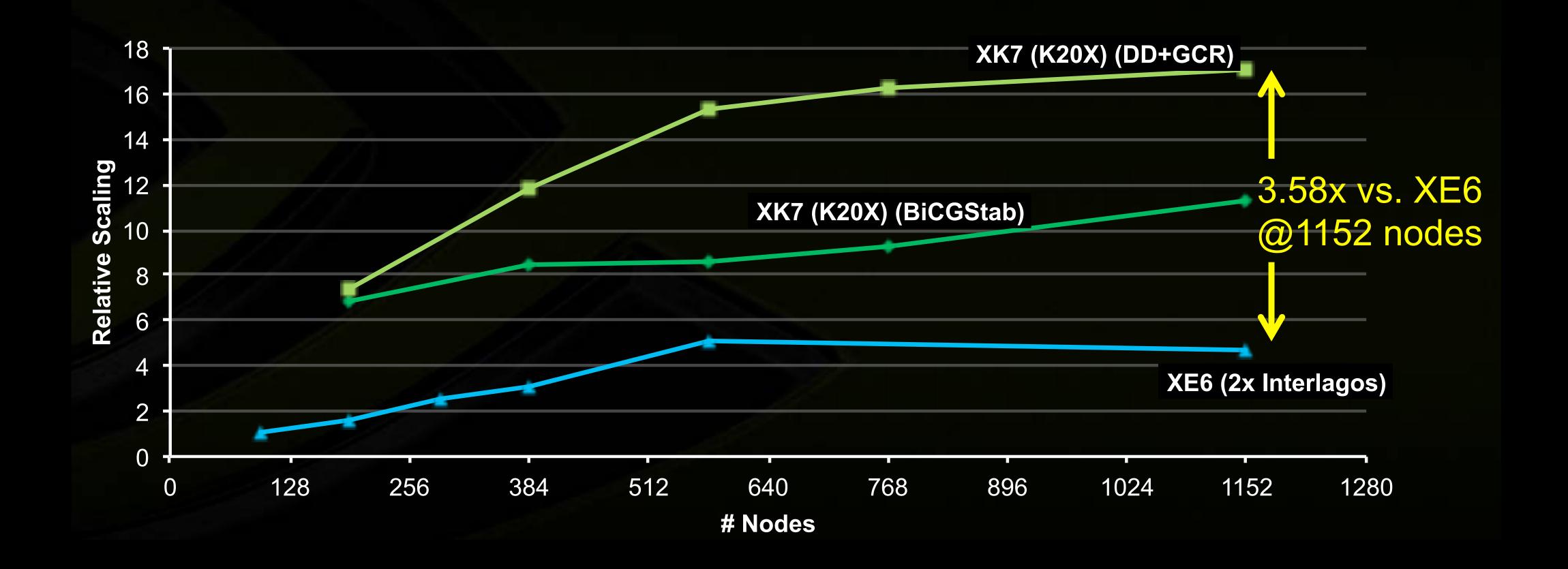
Strong Scaling Chroma with DD

Chroma

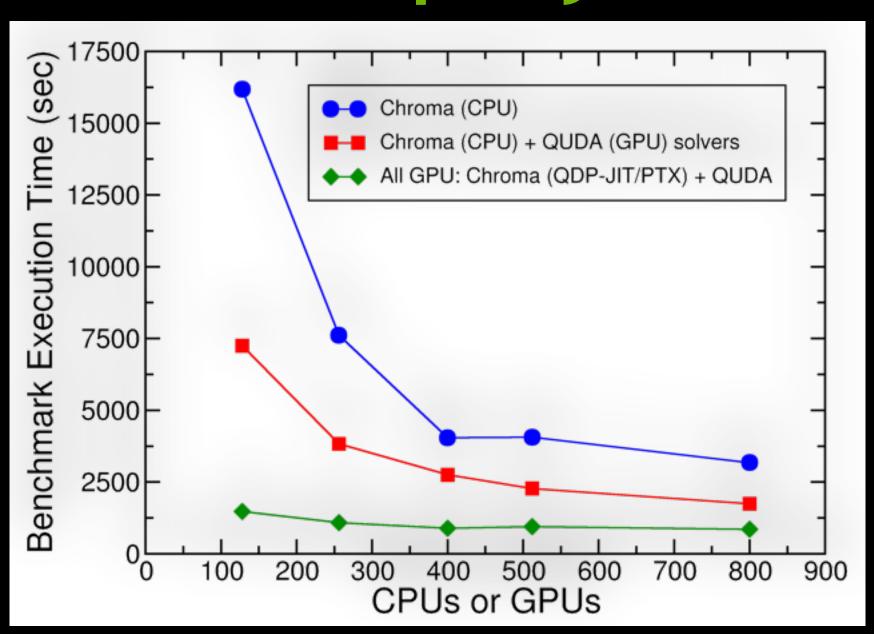
48³x512 lattice Relative Scaling (Application Time)

"XK7" node = XK7 (1x K20X + 1x Interlagos)

"XE6" node = XE6 (2x Interlagos)

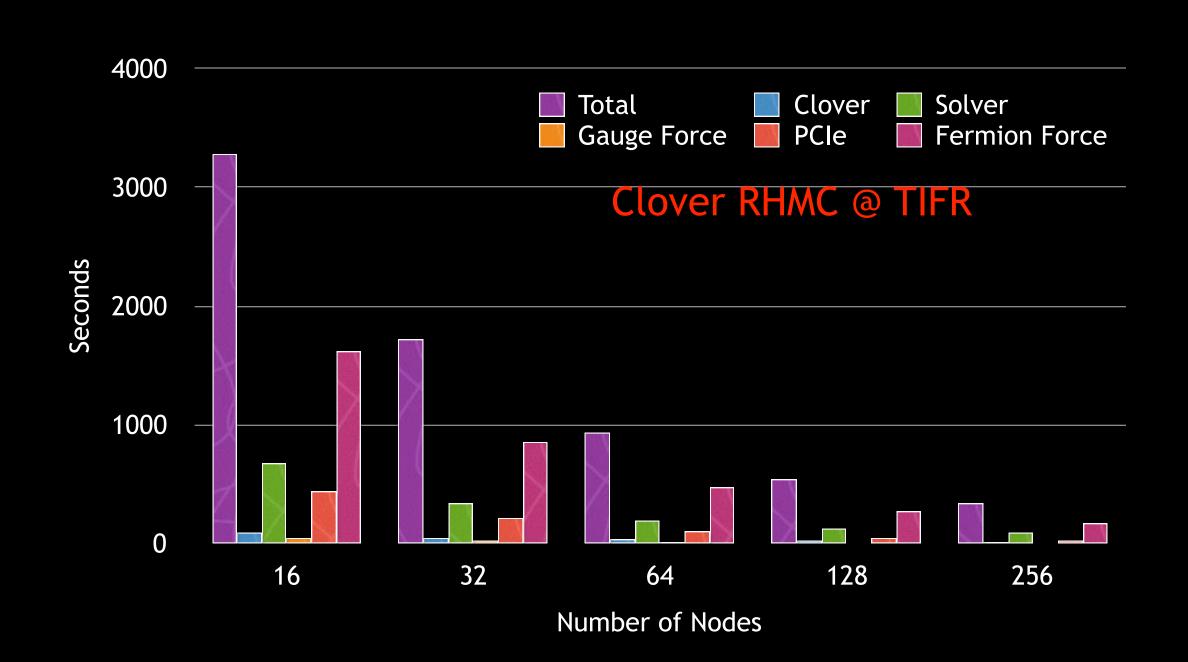


Wide deployment on GPU clusters



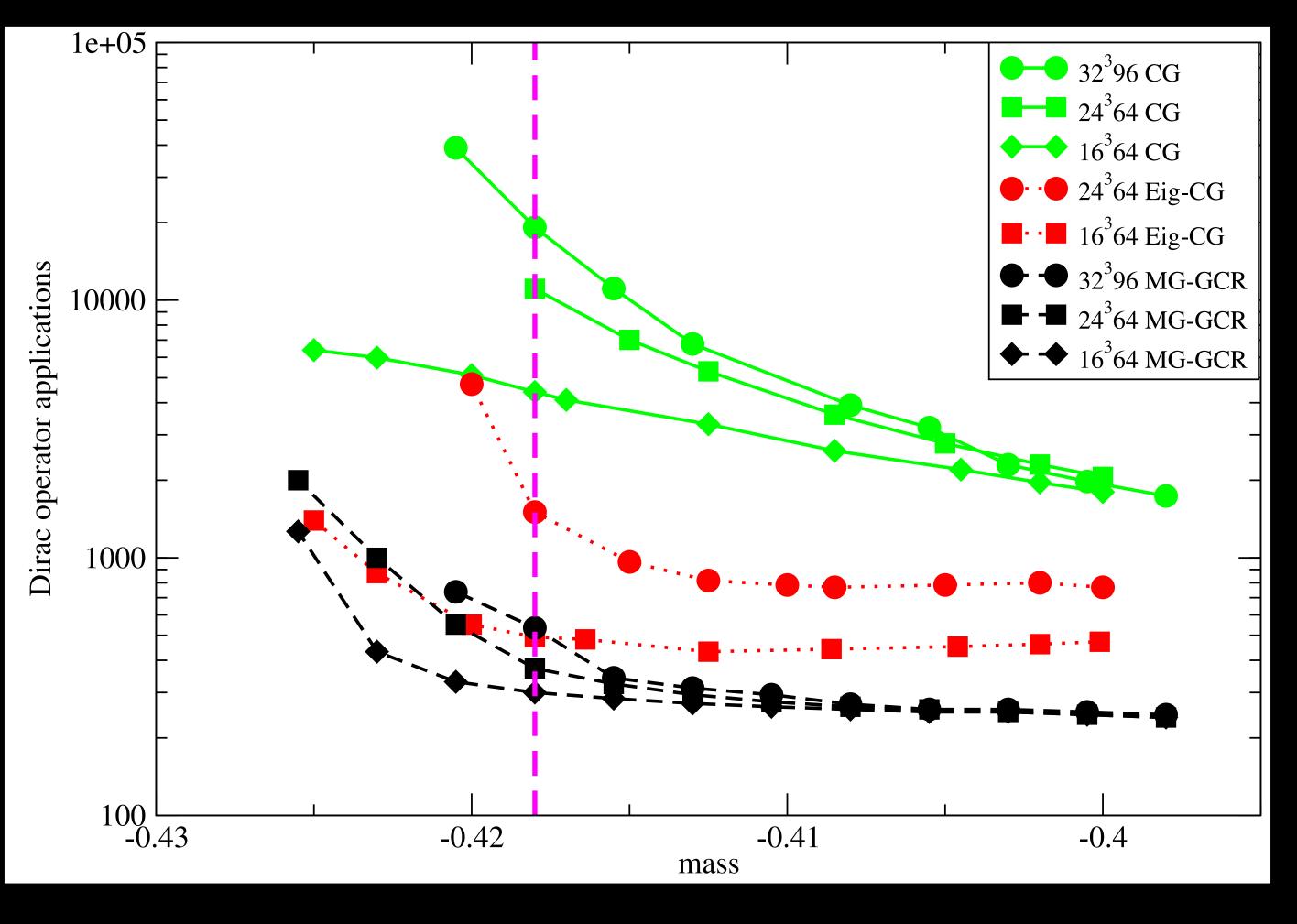
- Clover RHMC on Titan and Blue Waters (Chroma)
- Staggered RHMC @ FNAL (MILC)
- Nuclear physics @ Jlab (Chroma)

- Clover RHMC running @ TIFR (MILC)
- Thermodynamics @ TIFR
- Twisted-mass @ INFN
- etc.



MULTIGRID AND HIERARCHICAL ALGORITHMS

Why Multigrid?



240 vectors

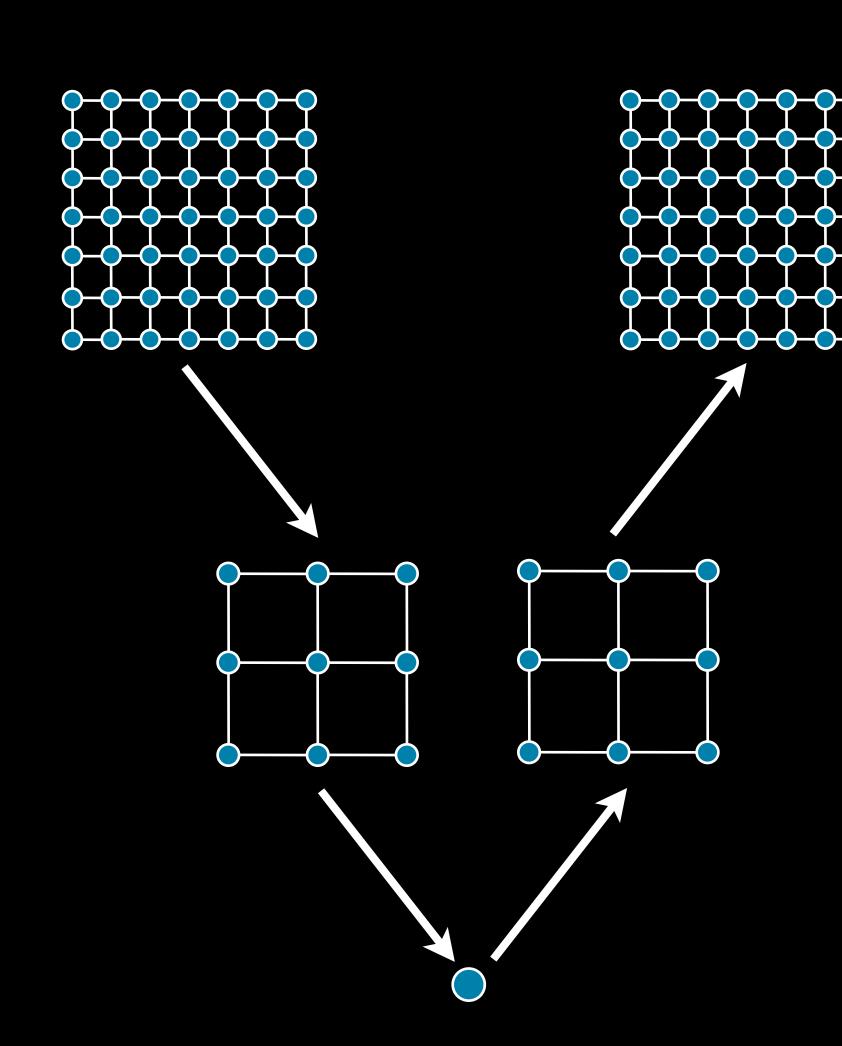
20 vectors

Babich et al 2010

Hierarchical algorithms for LQCD

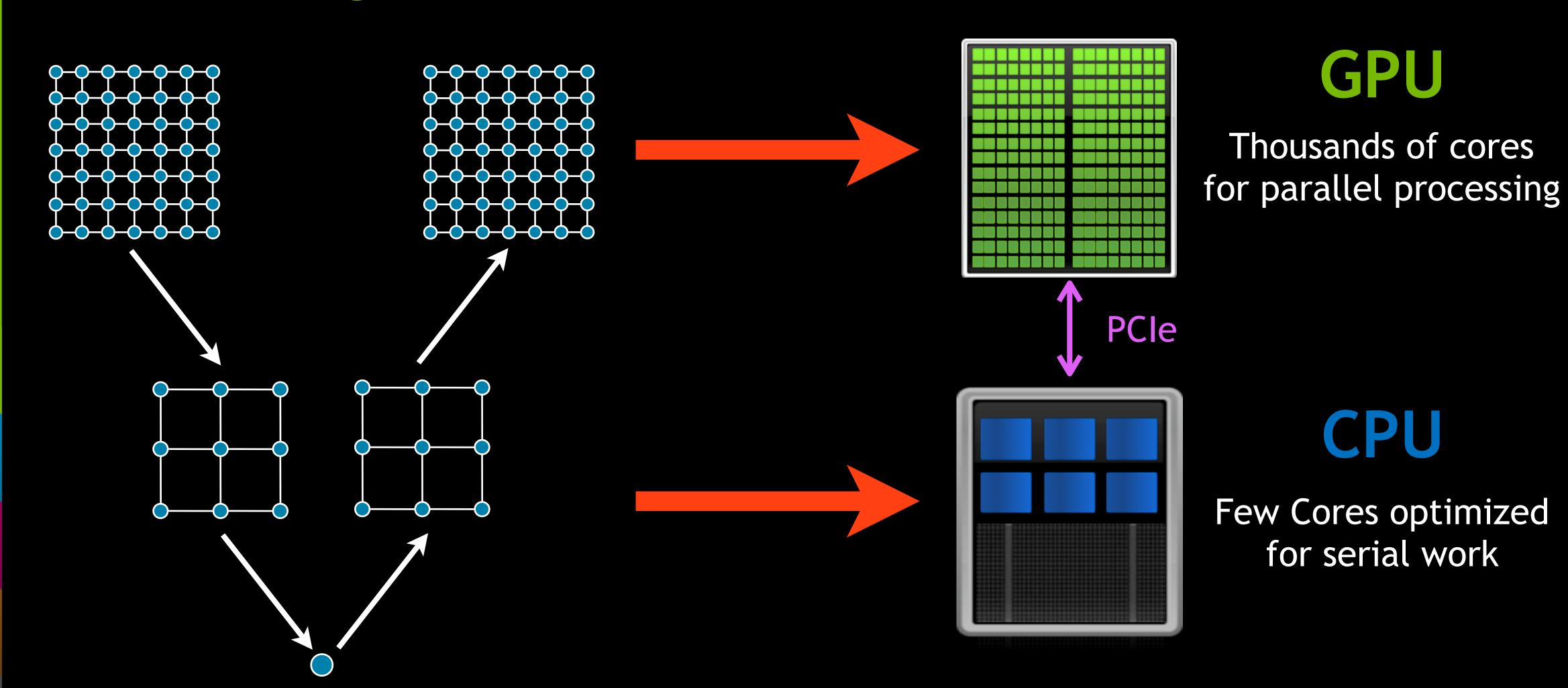
- Hierarchical algorithms have revolutionized LQCD computation
- Adaptive Geometric Multigrid for LQCD
 - Based on adaptive smooth aggregation (Brezina et al 2004)
 - Low modes have weak-approximation property => locally co-linear
 - Apply fixed geometric coarsening (Brannick et al 2007, Babich et al 2010)
- Clover Multigrid (Osborn et al 2010)
 - —Apply multigrid to the even/odd system
- Domain decomposition multigrid (Frommer et al 2012)
 - —Use Schwarz Alternating Procedure as smoother for improved scalability
- Inexact Deflation (Lüscher 2007)
 - Equivalent to adaptive "unsmoothed" aggregation
 - Local coherence = Weak-approximation property
 - —Uses an additive correction vs. MG's multiplicative correction
- Domain-wall Multigrid / Deflation (Cohen et al 2012, Boyle 2013)
 - —Apply to normal operator for positivity

The Challenge of Multigrid on GPU



- GPU requirements very different from CPU
 - Each thread is slow, but O(10,000) threads per GPU
- Fine grids run very efficiently
 - High parallel throughput problem
- Coarse grids are worst possible scenario
 - More cores than degrees of freedom
 - Increasingly serial and latency bound
 - Little's law (bytes = bandwidth * latency)
 - Amdahl's law limiter
- Multigrid exposes many of the problems expected at the Exascale
- Multigrid decomposes problem into throughput and latency parts

Hierarchical algorithms on heterogeneous architectures

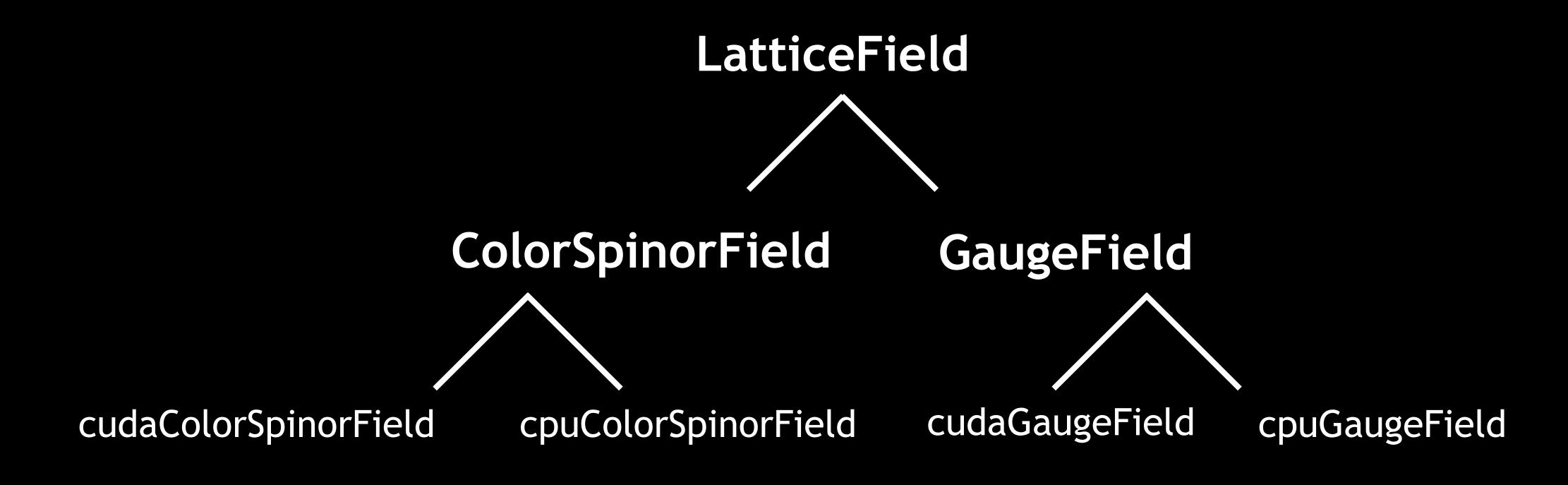


Design Goals

- Performance
 - LQCD typically reaches high % peak peak performance
 - Brute force can beat the best algorithm
 - Multigrid must be optimized to the same level
- Flexibility
 - Deploy level i on either CPU or GPU
 - All algorithmic flow decisions made at runtime
 - Autotune for a given heterogeneous
- (Short term) Provide optimal solvers to legacy apps
 - e.g., Chroma, CPS, MILC, etc.
- (Long term) Hierarchical algorithm toolbox
 - Little to no barrier to implementing new algorithms

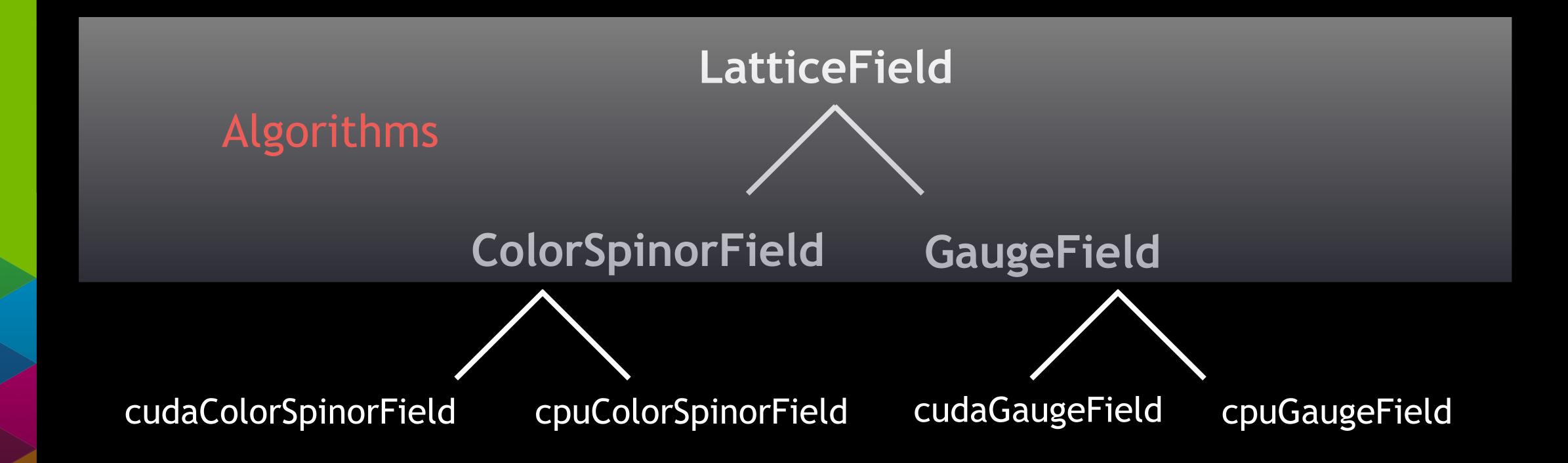
Multigrid and QUDA

QUDA designed to abstract algorithm from the heterogeneity



Multigrid and QUDA

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Multigrid and QUDA

QUDA designed to abstract algorithm from the heterogeneity

LatticeField



ColorSpinorField

GaugeField

cudaColorSpinorField

cpuColorSpinorField

cudaGaugeField

cpuGaugeField

Architecture

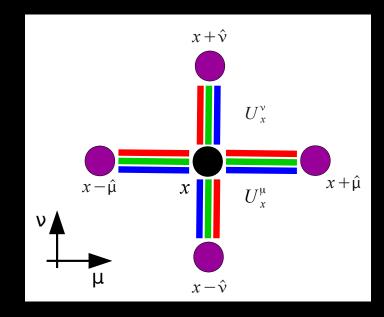
Writing the same code for two architectures

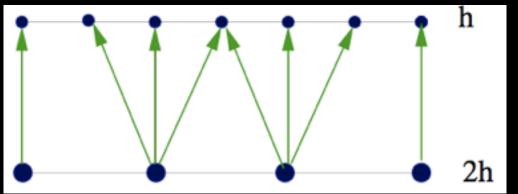
- Use C++ templates to abstract arch specifics
 - Load/store order, caching modifiers, precision, intrinsics

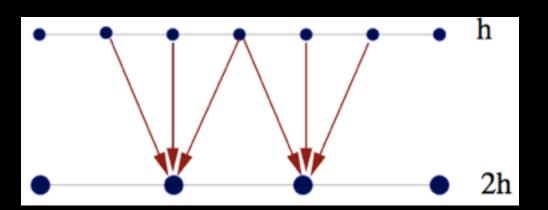
```
template<...> host device Real bar(Arg & arg, int x) {
                                   // do platform independent stuff here
                                   complex<Real> a[arg.length];
                                   arg.A.load(a);
platform specific load/store hidden here:
                                                                      platform independent stuff goes here
                                   ... // do computation
field order, cache modifiers, textures
                                                                      99% of computation goes here
                                   arg.A.save(a);
                                   return norm(a);
                                                               template<...> global void fooGPU(Arg arg) {
 template<...> void fooCPU(Arg &arg) {
                                                                 int tid = threadIdx.x + blockIdx.x*blockDim.x;
   arg.sum = 0.0;
                                                                 real sum = bar<...>(arg, tid);
 #pragma omp for
   for (int x=0; x<size; x++) platform specific parallelization
                                                                   shared__ typename BlockReduce::TempStorage tmp;
     arg.sum += bar<...>(arg, x);
                                                                 arg.sum = cub::BlockReduce<...>(tmp).Sum(sum);
                                    GPU: shared memory
                                    CPU: OpenMP, vectorization
      CPU
                                                                                           GPU
```

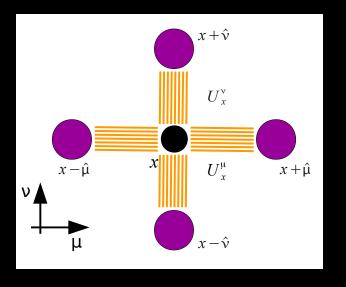
Ingredients for Parallel Adaptive Multigrid

- Prolongation construction (setup)
 - Block orthogonalization of null space vectors
 - Batched QR decomposition
- Smoothing (relaxation on a given grid)
 - Repurpose existing solvers (DD preconditioner)
- Prolongation
 - interpolation from coarse grid to fine grid
 - one-to-many mapping
- Restriction
 - restriction from fine grid to coarse grid
 - many-to-one mapping
- Coarse Operator construction (setup)
 - Evaluate R A P locally
 - Batched (small) dense matrix multiplication
- Coarse grid solver
 - direct solve on coarse grid?
 - (near) serial algorithm

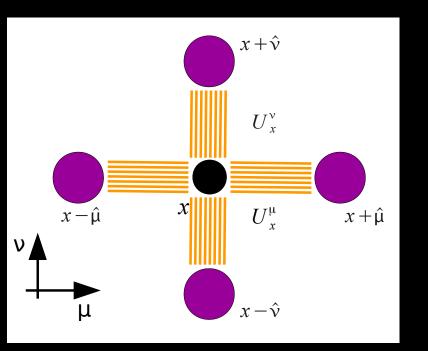








Coarse Grid Operator Analysis



- Coarse operator looks like a Dirac operator
 - Link matrices have dimension $2N_v \times 2N_v$ (e.g., 48 x 48)

$$\hat{D}_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'} = -\sum_{\mu} \left[Y_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}^{-\mu} \delta_{\mathbf{i}+\mu,\mathbf{j}} + Y_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}^{+\mu\dagger} \delta_{\mathbf{i}-\mu,\mathbf{j}} \right] + \left(M - X_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'} \right) \delta_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}$$

- Fine vs. Coarse grid parallelization
 - Fine grid operator has plenty of grid-level parallelism
 - E.g., $16^4 = 65536$ lattice sites
 - Coarse grid operator has diminishing grid-level parallelism
 - first coarse grid $4^4 = 256$ lattice sites
 - second coarse grid 2⁴ = 16 lattice sites
- Current GPUs have up to 3072 processing cores
- Need to consider finer-grained parallelization
 - Increase parallelism to use all GPU resources
 - Load balancing

Sources of Parallelism

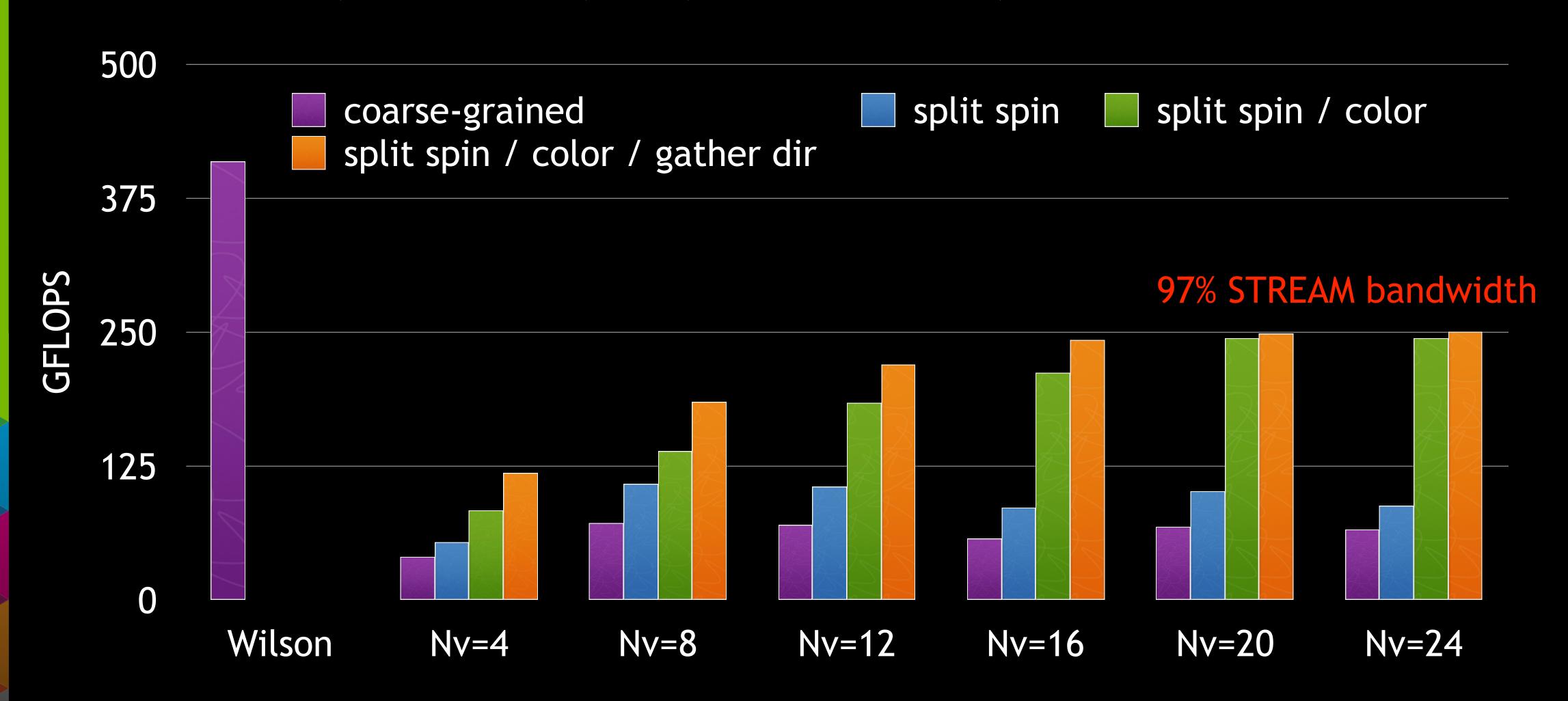
$$\hat{D}_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'} = -\sum_{\mu} \left[Y_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}^{-\mu} \delta_{\mathbf{i}+\mu,\mathbf{j}} + Y_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}^{+\mu\dagger} \delta_{\mathbf{i}-\mu,\mathbf{j}} \right] + \left(M - X_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'} \right) \delta_{\mathbf{i}\hat{s}\hat{c},\mathbf{j}\hat{s}'\hat{c}'}$$

- Site-level parallelism (i index)
 - Trivially data parallel
- Spin and color output index (s and c indices)
 - Trivially data parallel
- Stencil direction (µ index)
 - Loosely coupled parallelism (gather)
- Spin and color input index (s' and c' indices)
 - Tightly coupled parallelism (dot product)

$$2^4 => 24576$$
-way parallel $N_{\text{vec}=24}$

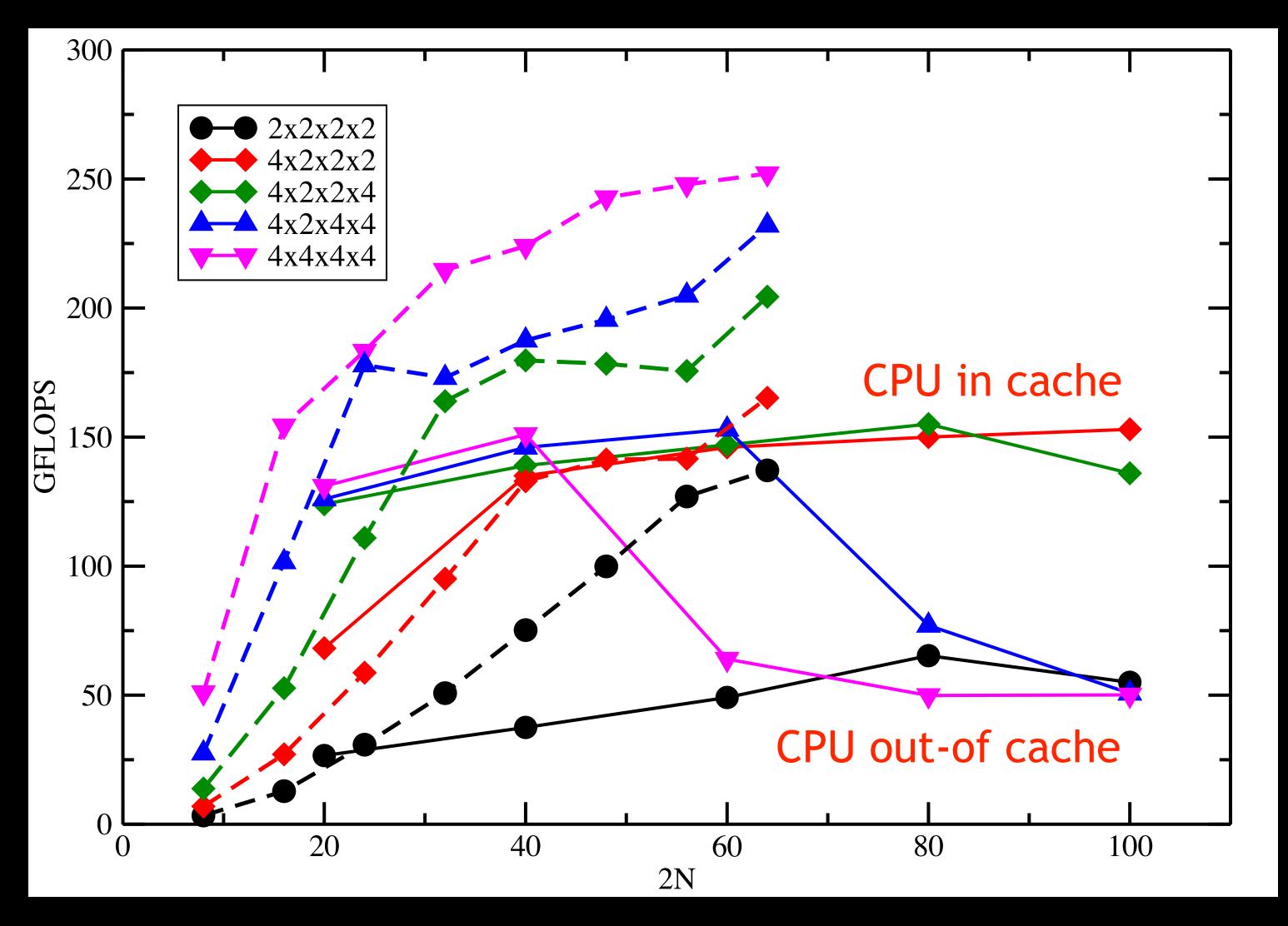
Coarse Grid Operator Performance

 $V_{\text{fine}} = 16^3 \text{x} 64$, $V_{\text{coarse}} = 4^3 \text{x} 16$, FP32, no reconstruction, Quadro M6000



Coarse Dslash Performance

8-core Haswell 2.4 GHz (solid line) vs M6000 (dashed lined)



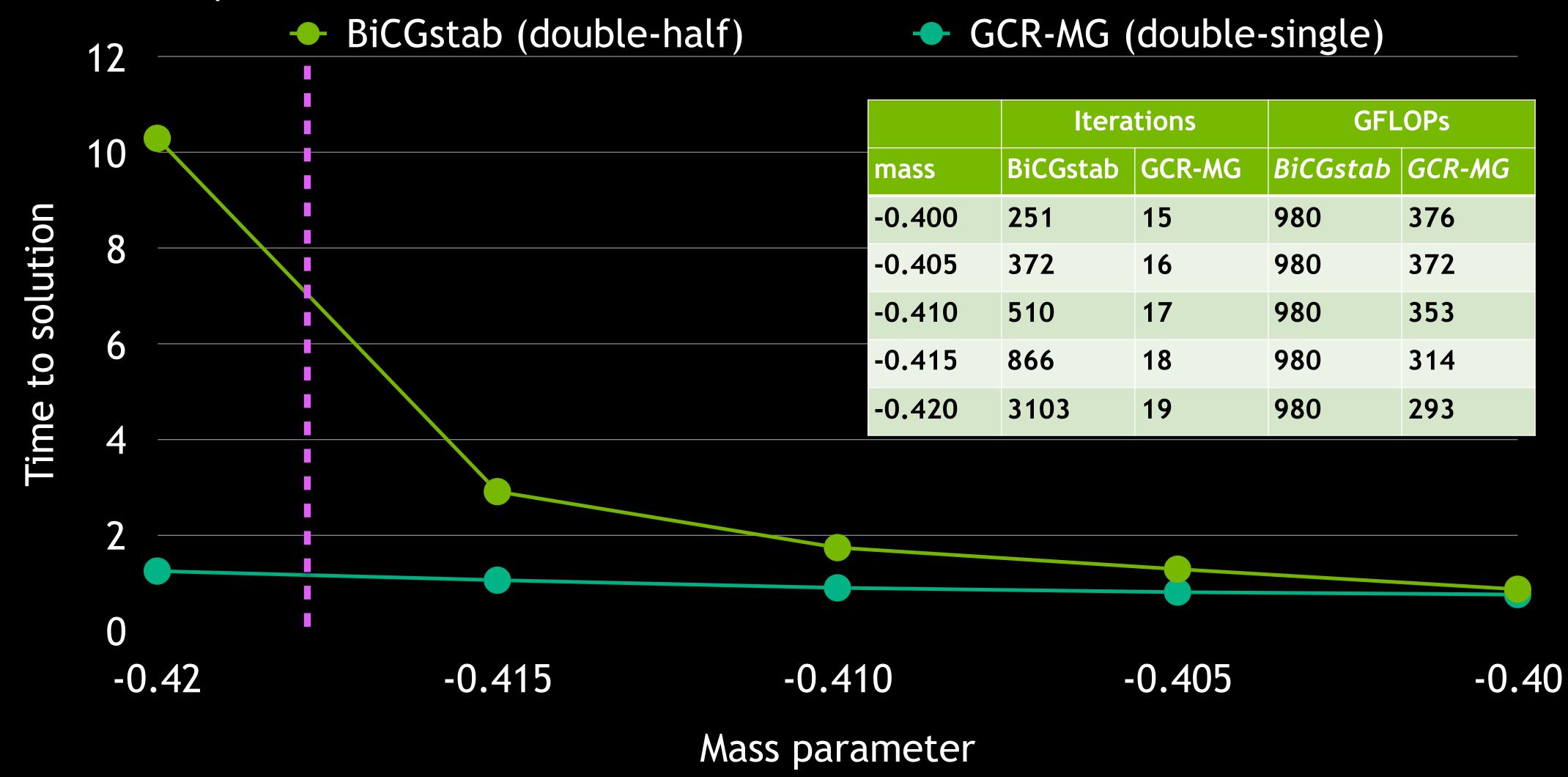
- Autotuner finds optimum degree of parallelization
 - Larger grids favor less fine grained
 - Coarse grids favor most fine grained
- GPU is nearly always faster than CPU
- Expect in future that coarse grids will favor CPUs
- For now, use GPU exclusively

Results

- Compare MG against the best traditional clover Krylov solver
 - BiCGstab in double/half precision
 - 12/8 reconstruct
 - Even-odd preconditioning
- Adaptive Multigrid algorithm
 - GCR outer solver wraps 3-level MG preconditioner
 - GCR restarts done in double, everything else in single
 - 24 or 32 null-space vectors on fine grid
 - Minimum Residual smoother
 - Even-odd preconditioning

Multigrid versus BiCGstab

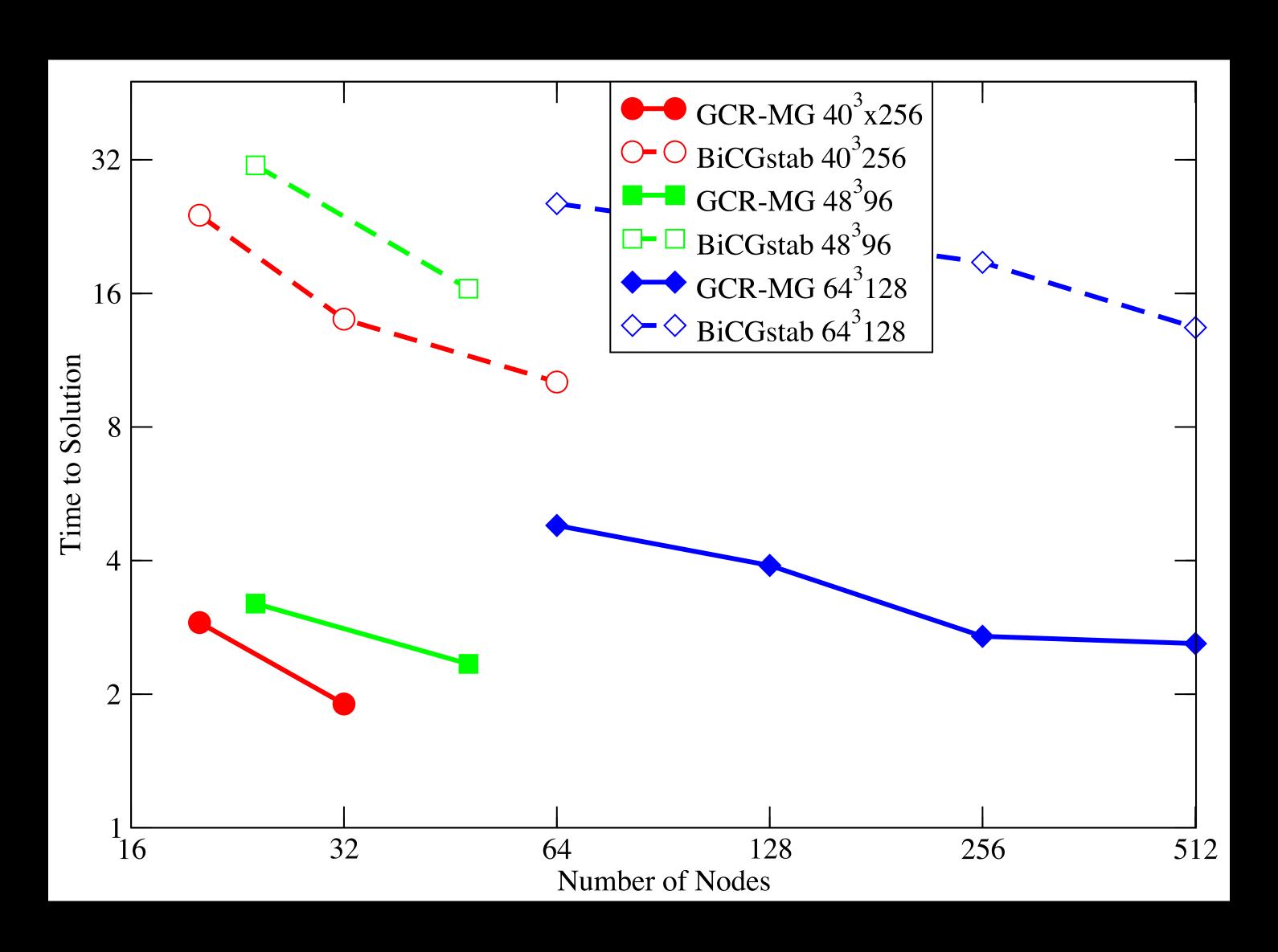
Anisotropic Wilson, V = 24³x64, 3x Quadro M6000



Multigrid vs BiCGstab Anisotropic Clover, $V = 40^3x256$, $m_{\pi} = 230$ MeV, light quark, 32 nodes of Titan

QUDA MG		QUDA BiCGStab		Speedup
Iterations	Time (sec)	Iterations	Time (sec)	
18	1.90	1811	17.98	9.46
18	1.89	1582	15.63	8.27
18	1.85	1613	16.02	8.66
19	2.02	1644	16.29	8.06
19	2.01	1788	17.67	8.79
18	1.90	1940	19.19	10.10
18	1.89	1568	15.58	8.24
19	2.00	1698	16.88	8.44
19	2.03	1914	18.98	9.35
18	1.85	1589	15.76	8.52
18	1.91	1735	17.16	8.98
Average	1.93		17.01	8.81

Titan Scaling Clover, $40^3x256\ 210\ m_\pi$, $48^3x96\ /\ 64^3x128\ 192\ MeV\ m_\pi$



Multigrid Summary and Future Work

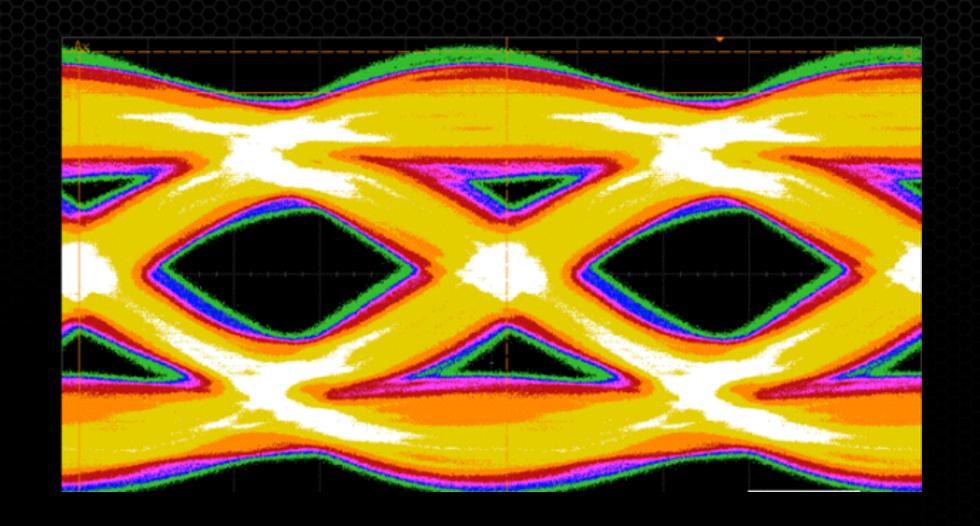
- Up to 10x speedups observed with multigrid
- Exploiting fine-grained parallelism was key
- Coarse solve dominates at large node count
- Lots more work to do
 - Strong scaling improvements
 - Absolute Performance tuning, e.g., half precision
 - Accelerate coarse grid solver: deflation or direct solve?
 - More flexible coarse grid distribution, e.g., redundant nodes
- Investigate off load coarse grids to the CPU
 - Use CPU and GPU simultaneously using additive MG
 - Likely optimal in the strong scaling limit

THE FUTURE

Introducing NVLINK and Stacked Memory

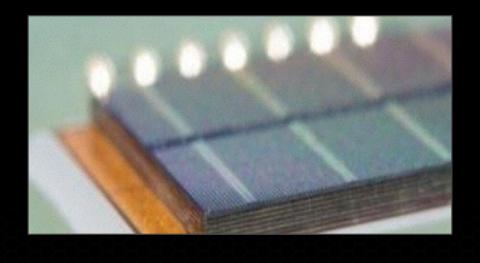
NVLINK

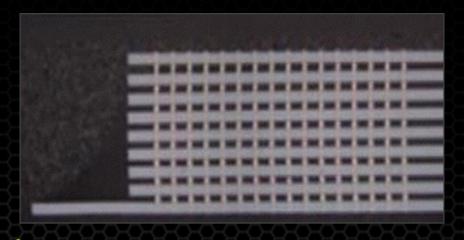
- GPU high speed interconnect
- 80-200 GB/s
- Planned support for POWER CPUs

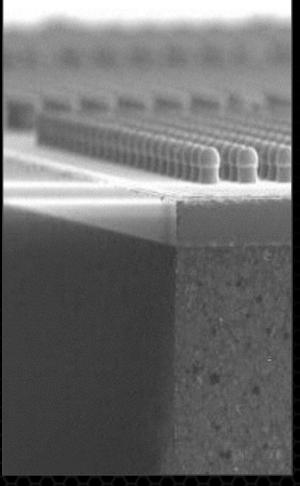


Stacked Memory

- 4x Higher Bandwidth (~1 TB/s)
- 3x Larger Capacity
- 4x More Energy Efficient per bit







Introduced with Pascal in 2016

GPU Computing in 2016

TESLA GPU NVLink 80 GB/s

CPU

HBM 1 Terabyte/s

Stacked Memory

DDR4 50-75 GB/s

DDR Memory

US to Build Two Flagship Supercomputers Powered by the Tesla Platform











100-300 PFLOPS Peak 10x in Scientific App Performance IBM POWER9 CPU + NVIDIA Volta GPU NVLink High Speed Interconnect 40 TFLOPS per Node, >3,400 Nodes 2017

Major Step Forward on the Path to Exascale

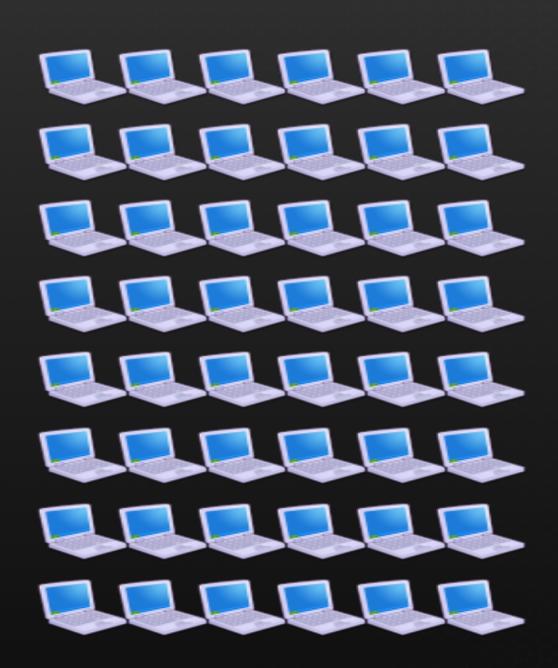




Just 4 nodes in Summit would make the Top500 list of supercomputers today



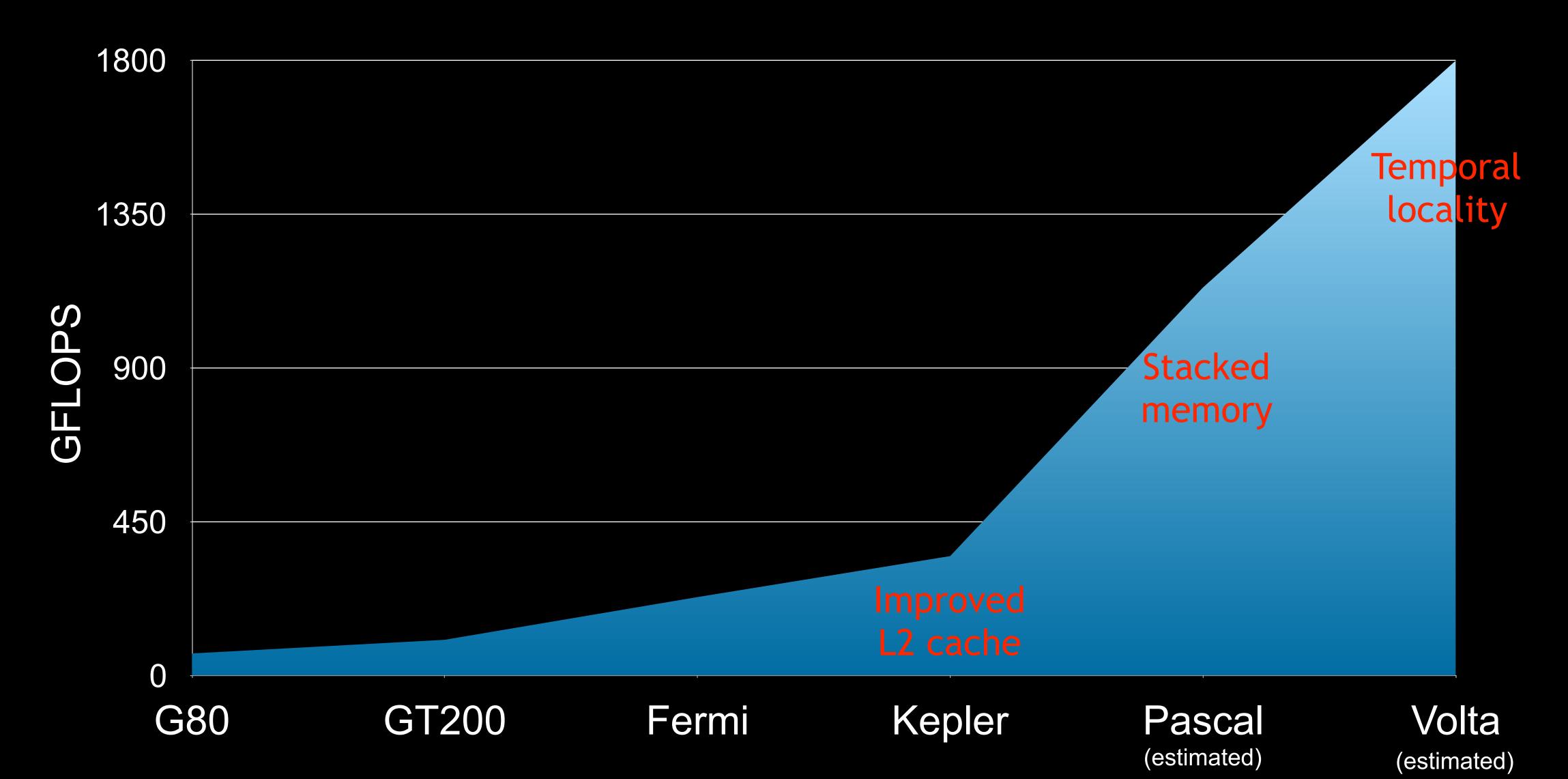
Similar Power as Titan
5-10x Faster
1/5th the Size



150 PF = 3M Laptops
One laptop for Every Resident in
State of Mississippi

LQCD Performance with GPU generation

Single Precision Wilson-Dslash performance, V=244

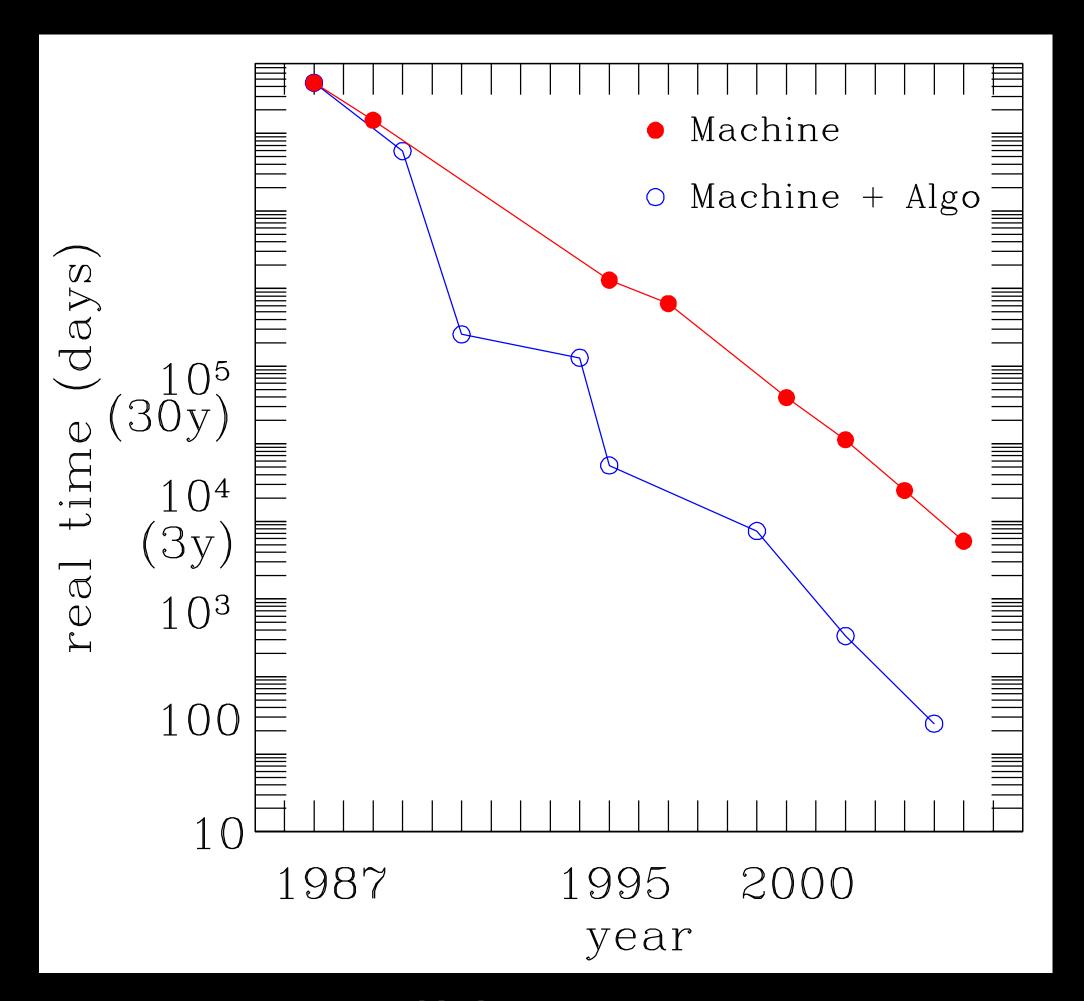


How to get to the Exascale (and beyond)?

- Four challenges to overcome
 - Communication
 - Latency
 - Parallelism
 - Locality
- What's the answer to all of the above?

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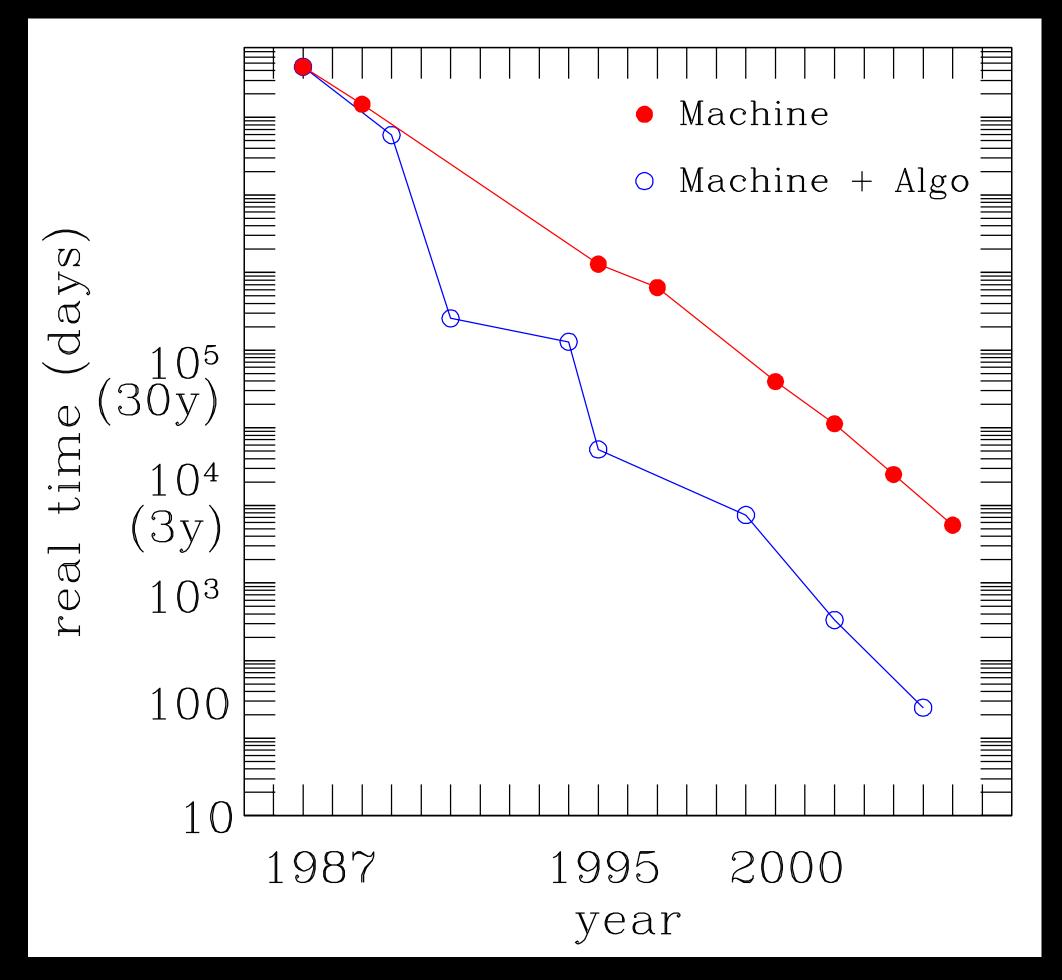
K Jansen

How to get to the Exascale (and beyond)?

- Four challenges to overcome
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Algorithms

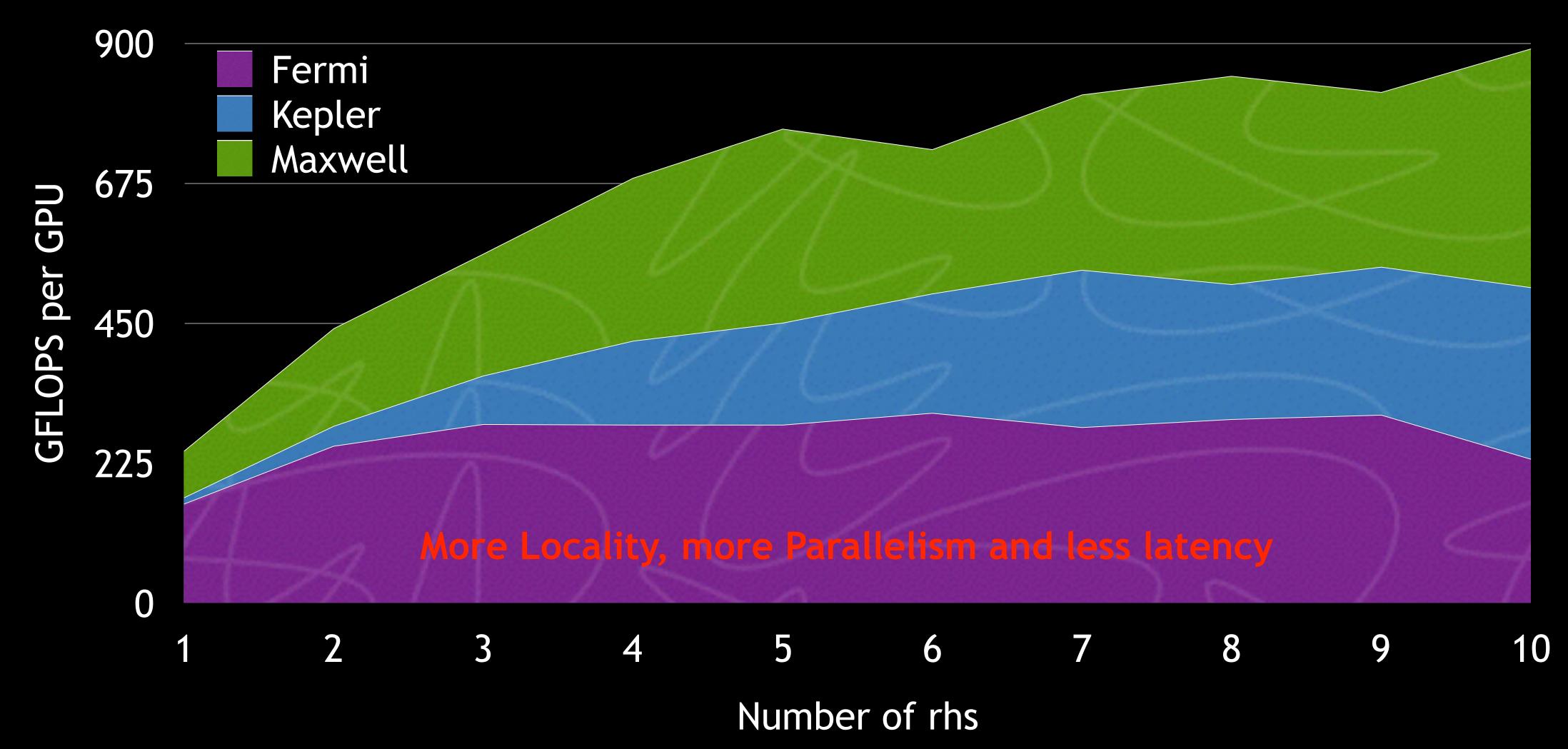
*and the ability to express and utilize those algorithms



K Jansen

Example: Multi-right-hand-side Dslash

Improved staggered, volume = 24⁴, single precision, no reconstruction



Software and Algorithms

- Solvers continue to innovate rapidly
 - Communication avoiding Krylov solvers (Demmel et al)
 - Cooperative Krylov methods (Bhaya et al)
 - Enlarged Krylov space methods (Grigori et al)
- Software can be the problem
 - Hierarchical grids breaks most LQCD frameworks
 - Used to calling solvers in a serial fashion
 - Precision is often baked in

Fine-grained Parallelism and the Implications for DSLs

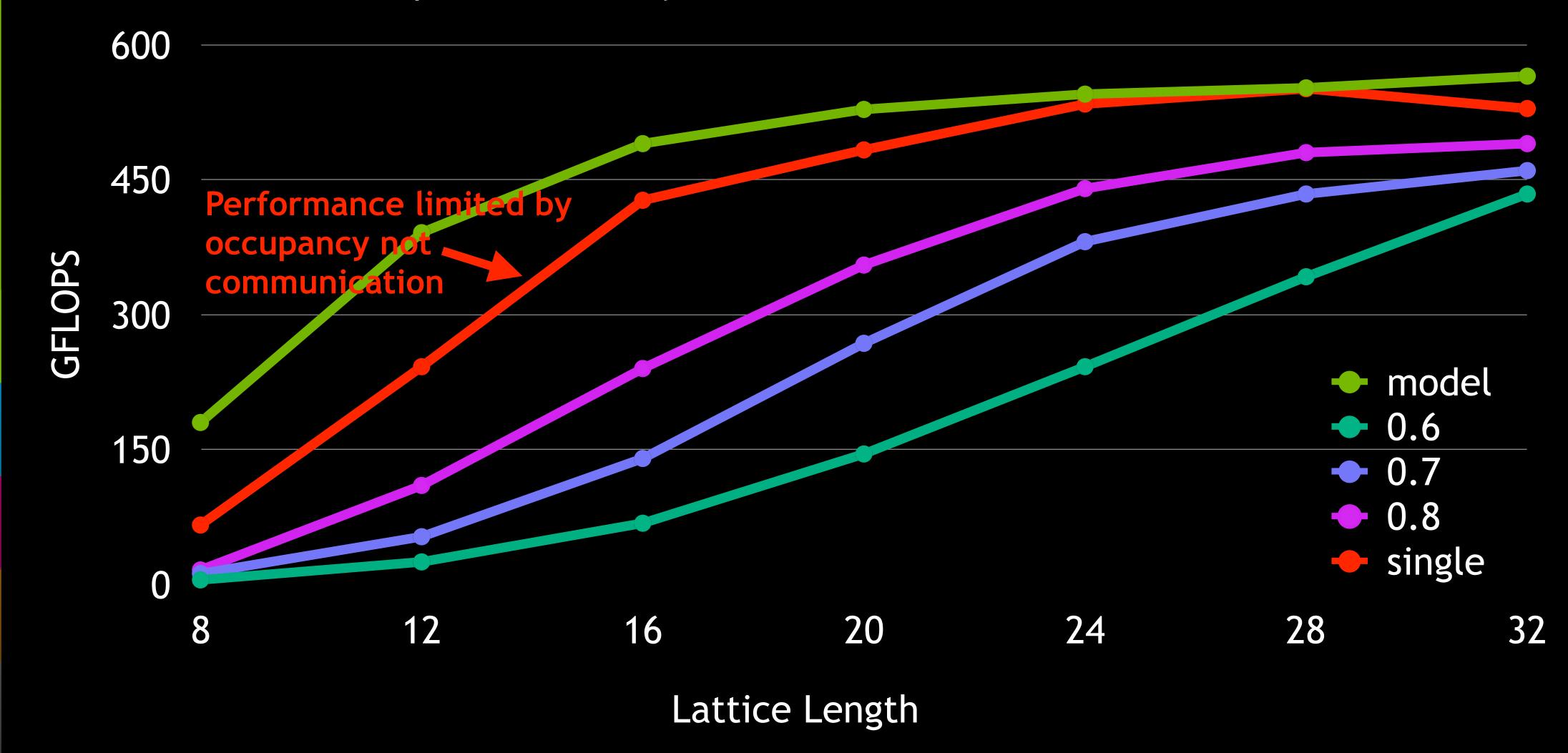
Traditional DSL approach is to abstract the grid parallelism

```
Matrix u;
Vector x, y;
y = u * x;
```

- Compiler / front end will then transform this expression into a data parallel operation using OpenMP / CUDA / C++ meta template magic, etc.
- This abstraction breaks with multigrid
 - Not enough grid parallelism
- Platform and algorithmic independent conjecture
 "Fine-grained parallelization will becoming increasingly a requirement at the Exascale (and beyond)"

Dslash Strong Scaling

K40, wilson, half precision, 8-way communication, 12 reconstruct



Communication at the Exascale

- Traditional two-sided MPI will not scale
 - Overheads will dominate communication
- Expect machine-wide unified address space
 - Every CPU/GPU can read/write directly to each other
 - SHMEM / UPC / MPI-3 everywhere
- Utilize the GPU's fine-grained latency hiding through thread oversubscription to hide inter-node latency
 - LQCD is an ideal application for this programming model
- QUDA is one of the applications being investigated in the DOE's "DesignForward" Exascale programming investigation

Conclusions and Outlook

GPUs provide a compelling platform for lattice computation

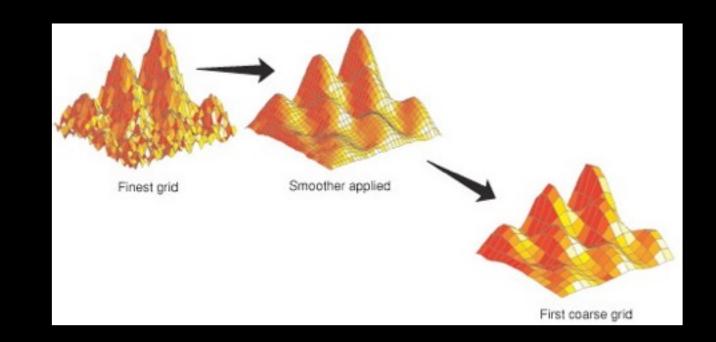
- Multigrid algorithms are running well on GPUs
 - Much more work to do
 - Fine-grained parallelization is key
 - Glimpse into the challenges of the exascale
- Importance of algorithms will only increase
- Exascale potentially challenging from a software point of view

Adaptive Geometric Multigrid

- Adaptively find candidate null-space vectors
 - Dynamically learn the null space and use this to define the prolongator
 - Algorithm is self learning



- 1. Set solver to be simple smoother
- 2. Apply current solver to random vector $v_i = P(D) \eta_i$
- 3. If convergence good enough, solver setup complete
- 4. Construct prolongator using fixed coarsening (1 P R) $v_k = 0$
 - → Typically use 4⁴ geometric blocks
 - ightharpoonup Preserve chirality when coarsening R = γ_5 P[†] γ_5 = P[†]
- 5. Construct coarse operator ($D_c = R D P$)
- 6. Recurse on coarse problem
- 7. Set solver to be augmented V-cycle, goto 2



Halo Region Updates (QUDA 0.7)

- Best way to reduce latency all round is kernel fusion
 - Reduces API calls
 - Reduces kernel launch overhead
 - Increases GPU occupancy
- Previous multi-GPU dslash had 6 kernels
 - pack (all faces), interior, halo_t, halo_z, halo_y, halo_x
- This puts a lower bound on the minimum time taken regardless of the speed of the GPU execution
- Fused multi-GPU dslash now has 3 kernels halving lower bound
 - pack (all faces), interior, halo (all faces)
- Scope for further fusing if we consider Deo Doe together
 - pack -> interior -> halo -> pack -> interior -> halo

Other improvements

- Double buffering of QMP/MPI receive buffers (QUDA 0.7)
 - Early pre-posting of MPI Receive
- Dslash has been rewritten using pthreads to parallelize between independent MPI and CUDA API calls (QUDA 0.8)
 - Parallelize between CUDA -> MPI and MPI -> CUDA dependent operations.
 E.g., waiting on MPI in t dimension while waiting on device -> host copy in z dimension
- Improvement to half-precision latency (QUDA 0.8)
 - Previously norm field was stored in separate halo region
 - Now store in same array as main quark field
 - Halves host -> device API calls
 - Increases message size for improved throughput

- GPU kernel / memcpy launch overhead (4-10 us)
 - Reduce number of kernels / memcpy
 - Use a single kernel for all halo regions (6->3 kernel calls) (0.7)

- GPU kernel / memcpy launch overhead (4-10 us)
 - Reduce number of kernels / memcpy
 - Use a single kernel for all halo regions (6->3 kernel calls) (0.7)
- Halo region kernels don't saturate the GPU
 - Use a single kernel for all halo regions (4x threads) (0.7)

- GPU kernel / memcpy launch overhead (4-10 us)
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- MPI / CUDA have to interact synchronously via CPU
 - GPU Direct Async coming with CUDA 8.0

Mixed-precision solvers

- QUDA has had mixed-precision from the get go
- Almost a free lunch where it works well (wilson/clover)
 - Residual injection / reliable updates mixed-precision BiCGstab
 - 2 Tflops sustained in workstation (4 GPUs)
- Did not work well for CG (staggered / twisted mass / dwf)
 - double-single has increased iteration count
 - double-half non convergent
- Why is this?
 - CG recurrence relations much more intolerant
 - BiCGstab noisy as hell anyway
- Need to make CG more robust
 - Make double-half work
 - Less polishing in mixed-precision multi-shift solver

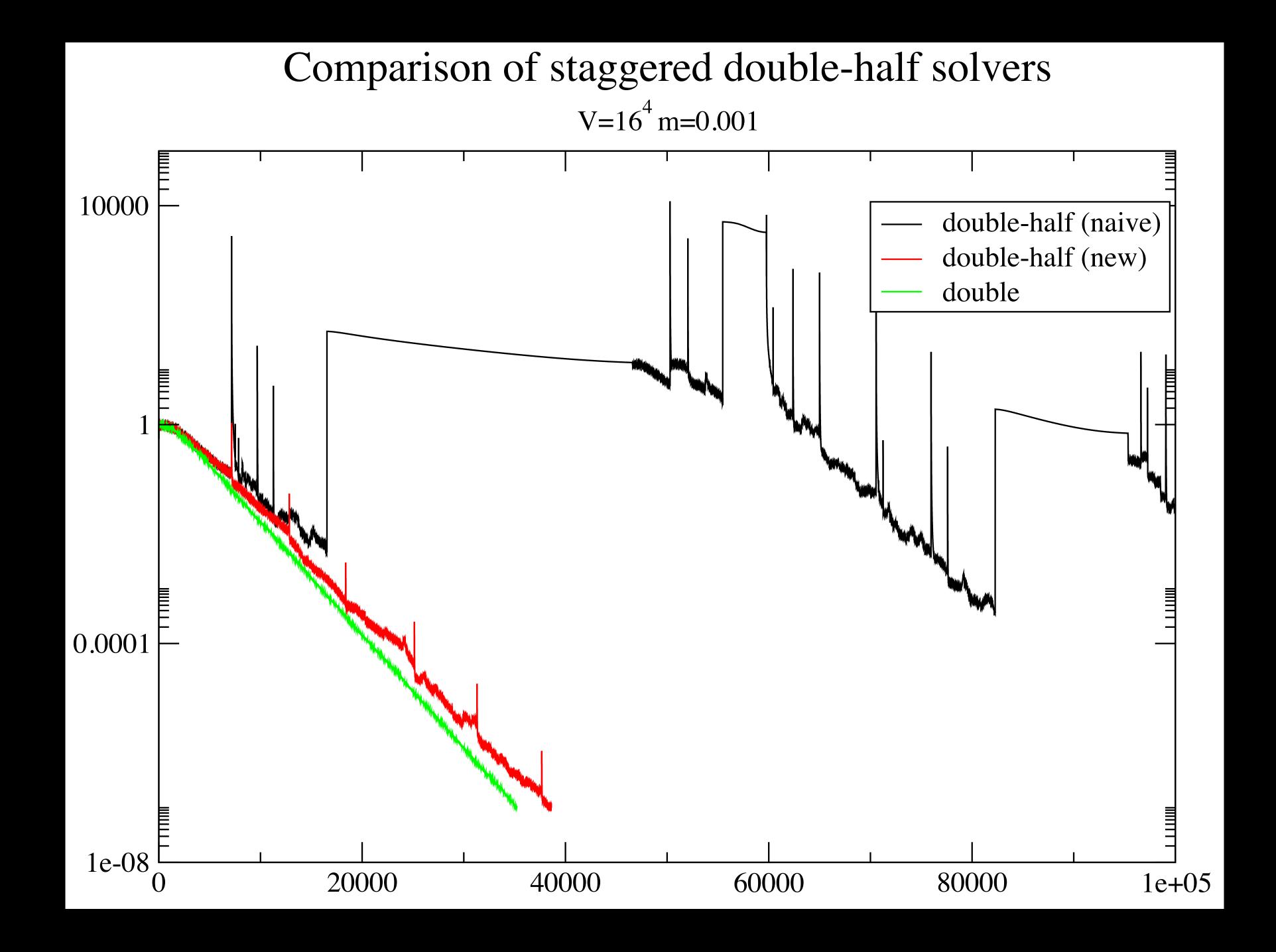
(Stable) Mixed-precision CG

- CG convergence relies on gradient vector being orthogonal to residual
 - Re-project when injecting new residual
- ullet α chosen to minimize $|e|_A$
 - True irrespective of precision of p, q, r
 - Solution correction is truncated if we keep low precision x
 - Always keep solution vector in high precision
- β computation relies on $(r_i,r_j) = |r_i|^2 \delta_{ij}$
 - Not true in finite precision
 - Polak-Ribière formula is equivalent and self-stabilizing through local orthogonality

$$\beta_k = \alpha(\alpha(q_k, q_k) - (p_k, q_k))/(r_{k-1}, r_{k-1})$$

- Further improvement possible
 - Mining the literature on fault-tolerant solvers...

```
while (|\mathbf{r}_{k}| > \epsilon) {
\beta_{k} = (\mathbf{r}_{k}, \mathbf{r}_{k})/(\mathbf{r}_{k-1}, \mathbf{r}_{k-1})
\mathbf{p}_{k+1} = \mathbf{r}_{k} - \beta_{k} \mathbf{p}_{k}
\mathbf{q}_{k+1} = A \mathbf{p}_{k+1}
\alpha = (\mathbf{r}_{k}, \mathbf{r}_{k})/(\mathbf{p}_{k+1}, \mathbf{q}_{k+1})
\mathbf{r}_{k+1} = \mathbf{r}_{k} - \alpha \mathbf{q}_{k+1}
\mathbf{x}_{k+1} = \mathbf{x}_{k} + \alpha \mathbf{p}_{k+1}
k = k+1
}
```



Multigrid vs BiCGstab Anisotropic Clover, $V = 40^3x256$, $m_{\pi} = 230$ MeV, strange quark, 32 nodes of Titan

QUDA MG		QUDA BiCGStab		Speedup
Iterations	Time (sec)	Iterations	Time (sec)	
12	1.74	178	2.19	1.25
12	1.74	167	2.04	1.18
12	1.74	186	2.24	1.29
12	1.77	163	2.01	1.13
12	1.74	171	2.04	1.18
12	1.74	184	2.26	1.29
12	1.75	173	2.09	1.19
12	1.73	161	1.94	1.12
12	1.74	179	2.20	1.26
12	1.73	208	2.53	1.46
12	1.73	163	1.97	1.14
12	1.74	169	2.06	1.19
Average	1.74		2.13	1.22

Linear Solvers

- QUDA supports a wide range of linear solvers
 - CG, BiCGstab, GCR, Multi-shift solvers, etc.
- As well as domain decomposition preconditioners
 - Additive/Multiplicative Schwarz, overlapping domains
- Together with almost all fermion actions under the sun
 - Wilson, Wilson-clover
 - Twisted mass, degenerate and non degenerate twisted mass
 - Twisted with a clover term
 - HISQ, ASQTAD, naive staggered
 - Domain wall, Möbius
- Condition number inversely proportional to mass
 - Light (realistic) masses are highly singular
 - Naive Krylov solvers suffer from critical slowing down at decreasing mass

```
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\mathbf{q}_{k+1} = A \mathbf{p}_{k+1}
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\mathbf{r}_{k+1} = \mathbf{r}_{k} - \alpha \mathbf{q}_{k+1}
\mathbf{x}_{k+1} = \mathbf{x}_{k} + \alpha \mathbf{p}_{k+1}
k = k+1
}
```

conjugate gradient

Coarse Grid Operator Performance

